Package: mdrb (via r-universe)

May 31, 2026

Title Metabodecon Rust Backend

Version 0.0.5

Description Provides a high-performance Rust backend for the 'metabodecon' package (<https://github.com/spang-lab/metabodecon>), enabling efficient deconvolution, alignment, and post-processing of 1-dimensional (1D) nuclear magnetic resonance (NMR) spectra. The package wraps optimized Rust functions to improve performance and scalability for large datasets. The recommended way to use *mdrb* is by installing *metabodecon* and setting the backend argument to `` `rust'' when calling its functions. The Rust part of the package is based on the 'metabodecon-rust' crate (<https://github.com/SombkeMaximilian/metabodecon-rust>).

License GPL (>= 3)

URL https://github.com/spang-lab/mdrb/, https://spang-lab.github.io/mdrb/

BugReports https://github.com/spang-lab/mdrb/issues

biocViews NMR, Deconvolution

Encoding UTF-8

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.2

Depends R (>= 4.2.0)

Suggests metabodecon, devtools, rextendr, testthat (>= 3.0.0)

Config/testthat/edition 3

Config/testthat/parallel true

BuildManual TRUE

Language en-US

Config/rextendr/version 0.3.1.9001

SystemRequirements Cargo (Rust's package manager), rustc (>= 1.80.0)

Config/pak/sysreqs libclang-dev

Repository https://spang-lab.r-universe.dev

Date/Publication 2026-05-31 00:43:27 UTC

RemoteUrl https://github.com/spang-lab/mdrb

RemoteRef HEAD

RemoteSha 5d293b2d69136c0657fdb356fc83cf904b0cccb9

Contents

`Deconvoluter` *Deconvoluter Class*

Description

Environment containing methods for the Deconvoluter class.

Usage

```
Deconvoluter
```

Format

An object of class `environment` of length 19.

Methods

```
x <- Deconvoluter$new()
x$add_ignore_region(start, end)
x$clear_ignore_regions()
x$clear_threads()
x$deconvolute_spectra(spectra)
x$deconvolute_spectrum(spectrum)
x$fitting_settings()
x$ignore_regions()
x$optimize_settings(reference)
x$par_deconvolute_spectra(spectra)
x$par_deconvolute_spectrum(spectrum)
x$selection_settings()
x$set_analytical_fitter(iterations)
x$set_detector_only()
```

```
x$set_identity_smoother()
x$set_moving_average_smoother(iterations, window_size)
x$set_noise_score_selector(threshold)
x$set_threads(threads)
x$smoothing_settings()
```

For more information on the methods, see the Rust documentation at https://github.com/SombkeMaximilian/metabodecon-rust.

`Deconvolution` *Deconvolution Class*

Description

Environment containing methods for the Deconvolution class.

Usage

```
Deconvolution
```

Format

An object of class `environment` of length 9.

Methods

```
# Assuming x is an object of class Deconvolution
x$lorentzians()
x$mse()
x$par_superposition_vec(chemical_shifts)
x$read_bin(path)
x$read_json(path)
x$superposition(chemical_shift)
x$superposition_vec(chemical_shifts)
x$write_bin(path)
x$write_json(path)
```

For more information on the methods, see the Rust documentation at https://github.com/SombkeMaximilian/metabodecon-rust.

Lorentzian *Lorentzian Class*

Description

Environment containing methods for the Lorentzian class.

Usage

```
Lorentzian
```

Format

An object of class `environment` of length 12.

Methods

```
x <- Lorentzian$new(sf, hw, maxp)
x$evaluate(x)
x$evaluate_vec(x)
x$hw()
x$maxp()
x$par_superposition_vec(x, sf, hw, maxp)
x$set_hw(hw)
x$set_maxp(maxp)
x$set_sf(sf)
x$sf()
x$superposition(x, sf, hw, maxp)
x$superposition_vec(x, sf, hw, maxp)
```

For more information on the methods, see the Rust documentation at https://github.com/SombkeMaximilian/metabodecon-rust.

Spectrum *Spectrum Class*

Description

Environment containing methods for the Spectrum class.

Usage

```
Spectrum
```

Format

An object of class `environment` of length 18.

Methods

```
x <- Spectrum$new(chemical_shifts, intensities, signal_boundaries)
x$chemical_shifts()
x$frequency()
x$intensities()
x$nucleus()
x$read_bin(path)
x$read_bruker(path, experiment, processing, signal_boundaries)
x$read_bruker_set(path, experiment, processing, signal_boundaries)
x$read_jcampdx(path, signal_boundaries)
x$read_json(path)
x$reference_compound()
x$set_frequency(frequency)
x$set_nucleus(nucleus)
x$set_reference_compound(reference)
x$set_signal_boundaries(signal_boundaries)
x$signal_boundaries()
x$write_bin(path)
x$write_json(path)
```

For more information on the methods, see the Rust documentation at https://github.com/SombkeMaximilian/metabodecon-rust.

Index